



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 30, 2020 – 02:09 PM EST

PDB ID : 6V8X
EMDB ID: : EMD-21111
Title : VRC01 Bound BG505 F14 HIV-1 SOSIP Envelope Trimer Structure
Authors : Henderson, R.; Acharya, P.
Deposited on : 2019-12-12
Resolution : 3.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

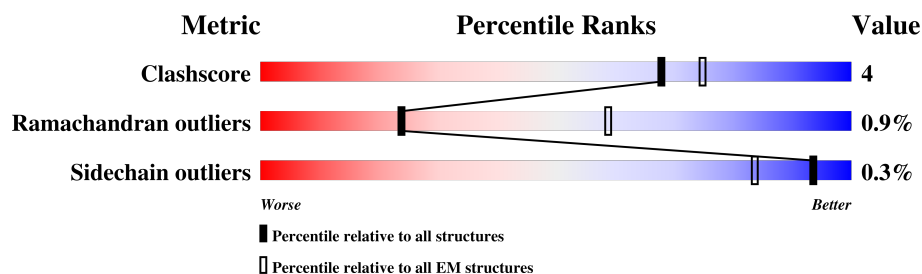
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	471	82% 11% • 7%
1	E	471	83% 10% • 7%
1	I	471	82% 11% • 7%
2	B	145	81% 7% 12%
2	F	145	81% 7% 12%
2	J	145	81% 7% 12%
3	C	224	92% 8% •
3	G	224	91% 8% •
3	K	224	92% 7% •

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Mol	Chain	Length	Quality of chain
4	D	208	<div><div></div><div>91%</div><div>7% •</div></div>
4	H	208	<div><div></div><div>92%</div><div>7% •</div></div>
4	L	208	<div><div></div><div>91%</div><div>7% •</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24825 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3453	2172	609	645	27		
1	E	439	Total	C	N	O	S	0	0
			3453	2172	609	645	27		
1	I	439	Total	C	N	O	S	0	0
			3453	2172	609	645	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ILE	VAL	conflict	UNP Q2N0S6
A	148	ALA	ASN	conflict	UNP Q2N0S6
A	204	VAL	ALA	conflict	UNP Q2N0S6
A	208	LEU	VAL	conflict	UNP Q2N0S6
A	255	LEU	VAL	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
E	68	ILE	VAL	conflict	UNP Q2N0S6
E	148	ALA	ASN	conflict	UNP Q2N0S6
E	204	VAL	ALA	conflict	UNP Q2N0S6
E	208	LEU	VAL	conflict	UNP Q2N0S6
E	255	LEU	VAL	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
I	68	ILE	VAL	conflict	UNP Q2N0S6
I	148	ALA	ASN	conflict	UNP Q2N0S6
I	204	VAL	ALA	conflict	UNP Q2N0S6
I	208	LEU	VAL	conflict	UNP Q2N0S6
I	255	LEU	VAL	conflict	UNP Q2N0S6
I	332	ASN	THR	conflict	UNP Q2N0S6
I	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	128	Total	C	N	O	S	0	0
			1025	649	178	192	6		
2	F	128	Total	C	N	O	S	0	0
			1025	649	178	192	6		
2	J	128	Total	C	N	O	S	0	0
			1025	649	178	192	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S9
F	605	CYS	THR	conflict	UNP Q2N0S9
J	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called VRC01 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	224	Total	C	N	O	S	0	0
			1710	1077	297	325	11		
3	G	224	Total	C	N	O	S	0	0
			1710	1077	297	325	11		
3	K	224	Total	C	N	O	S	0	0
			1710	1077	297	325	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	211	ALA	VAL	conflict	UNP Q6N095
G	211	ALA	VAL	conflict	UNP Q6N095
K	211	ALA	VAL	conflict	UNP Q6N095

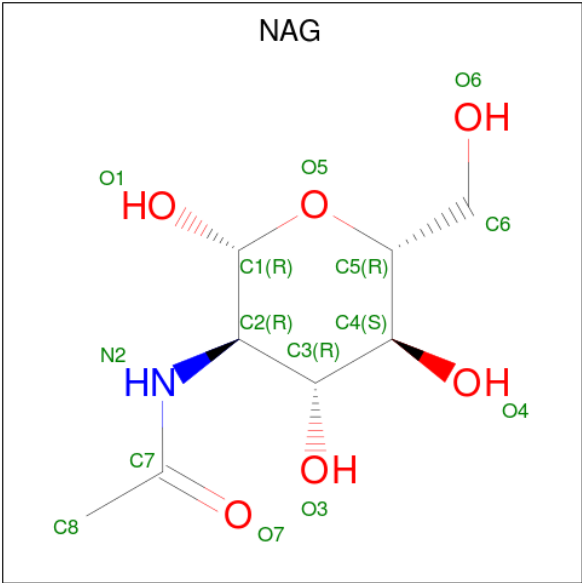
- Molecule 4 is a protein called VRC01 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1615	1011	277	322	5		
4	H	208	Total	C	N	O	S	0	0
			1615	1011	277	322	5		
4	L	208	Total	C	N	O	S	0	0
			1615	1011	277	322	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	204	ARG	SER	conflict	UNP Q6PIL8
H	204	ARG	SER	conflict	UNP Q6PIL8
L	204	ARG	SER	conflict	UNP Q6PIL8

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	A	1	Total	C	N	O	0
			392	224	28	140	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	

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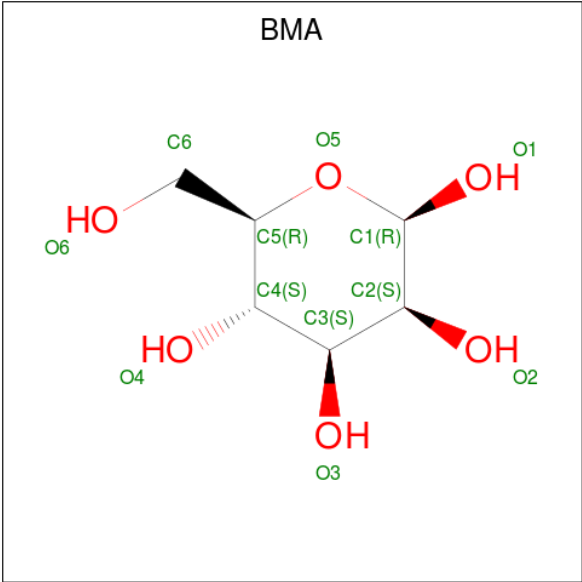
Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	E	1	Total	C	N	O	0
			392	224	28	140	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	

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Mol	Chain	Residues	Atoms				AltConf
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	I	1	Total	C	N	O	0
			392	224	28	140	
5	J	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



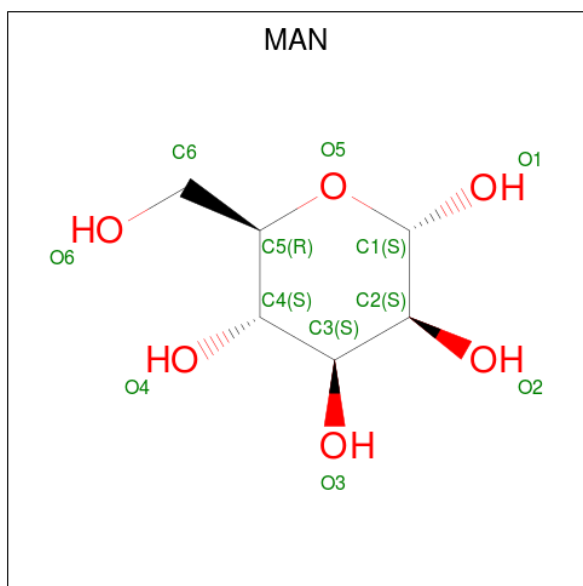
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	A	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	E	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	
6	I	1	Total	C	O	0
			55	30	25	

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Mol	Chain	Residues	Atoms			AltConf
6	I	1	Total	C	O	0
			55	30	25	

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

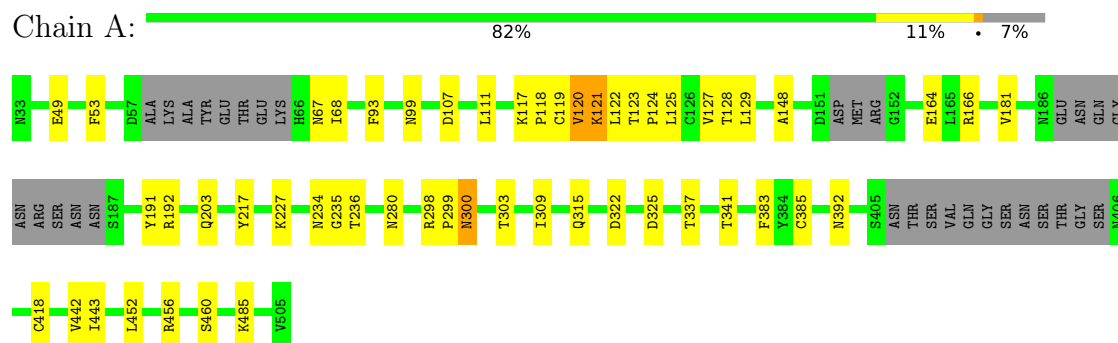


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			11	6	5	
7	E	1	Total	C	O	0
			11	6	5	
7	I	1	Total	C	O	0
			11	6	5	

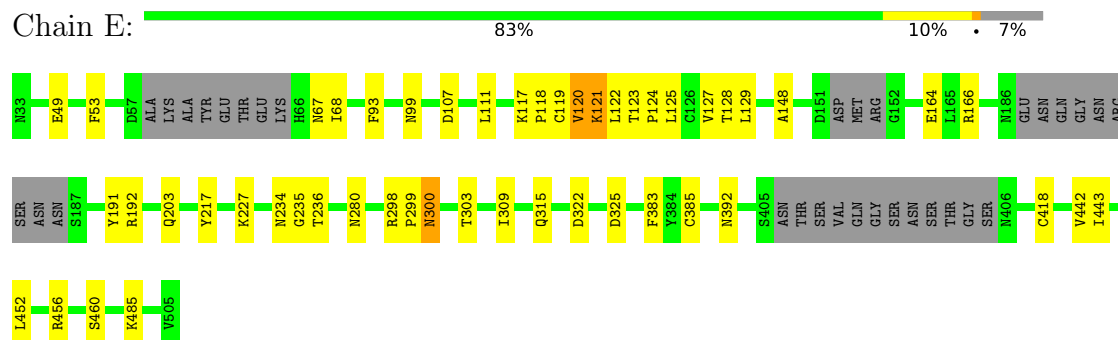
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

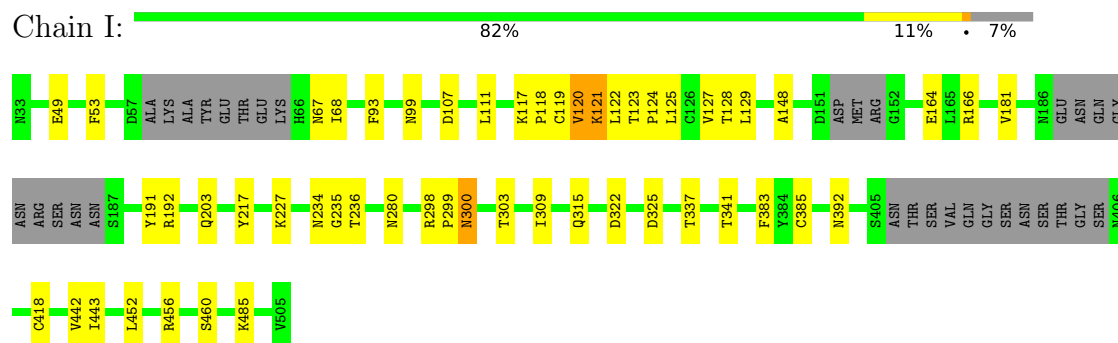
- Molecule 1: Envelope glycoprotein gp120




- Molecule 1: Envelope glycoprotein gp120

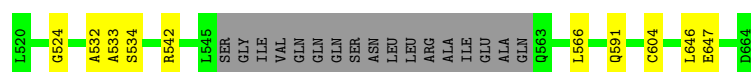


- Molecule 1: Envelope glycoprotein gp120




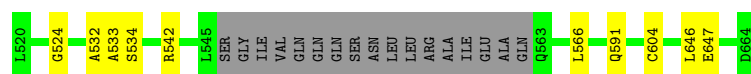
- Molecule 2: Envelope glycoprotein gp41

Chain B:  81% 7% 12%




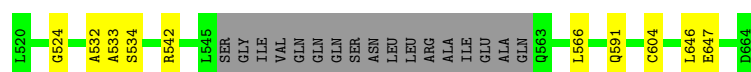
- Molecule 2: Envelope glycoprotein gp41

Chain F:  81% 7% 12%



- Molecule 2: Envelope glycoprotein gp41

Chain J:  81% 7% 12%




- Molecule 3: VRC01 Fab Heavy Chain

Chain C:  92% 8% .



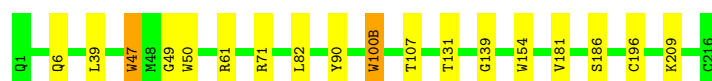
- Molecule 3: VRC01 Fab Heavy Chain

Chain G:  91% 8% .



- Molecule 3: VRC01 Fab Heavy Chain

Chain K:  92% 7% .



- Molecule 4: VRC01 Fab Light Chain

Chain D:  91% 7% .

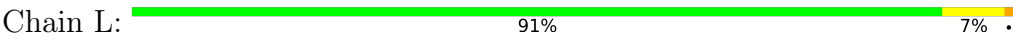


- Molecule 4: VRC01 Fab Light Chain

Chain H:  92% 7% .



● Molecule 4: VRC01 Fab Light Chain



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	77632	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
1	E	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
1	I	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
2	B	0.80	1/1043 (0.1%)	0.81	0/1414
2	F	0.80	1/1043 (0.1%)	0.81	0/1414
2	J	0.81	1/1043 (0.1%)	0.81	0/1414
3	C	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
3	G	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
3	K	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
4	D	0.61	0/1652	0.70	1/2242 (0.0%)
4	H	0.61	0/1652	0.70	1/2242 (0.0%)
4	L	0.61	0/1652	0.70	1/2242 (0.0%)
All	All	0.83	21/23922 (0.1%)	0.78	27/32481 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	H	0	1
4	L	0	1
All	All	0	3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	50	TRP	CB-CG	-11.02	1.30	1.50
3	K	50	TRP	CB-CG	-11.02	1.30	1.50
3	C	50	TRP	CB-CG	-11.01	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	299	PRO	N-CD	7.37	1.58	1.47
1	A	299	PRO	N-CD	7.30	1.58	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	88	CYS	CA-CB-SG	6.31	125.35	114.00
4	L	88	CYS	CA-CB-SG	6.31	125.35	114.00
4	H	88	CYS	CA-CB-SG	6.30	125.35	114.00
1	A	129	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	129	LEU	CA-CB-CG	6.19	129.53	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	90	GLN	Peptide
4	H	90	GLN	Peptide
4	L	90	GLN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3453	0	3397	48	0
1	E	3453	0	3397	46	0
1	I	3453	0	3397	49	0
2	B	1025	0	1012	4	0
2	F	1025	0	1012	4	0
2	J	1025	0	1012	4	0
3	C	1710	0	1680	8	0
3	G	1710	0	1680	9	0
3	K	1710	0	1680	8	0
4	D	1615	0	1554	12	0
4	H	1615	0	1554	11	0
4	L	1615	0	1554	12	0
5	A	392	0	347	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	0	0
5	E	392	0	347	2	0
5	F	14	0	13	0	0
5	I	392	0	347	1	0
5	J	14	0	13	0	0
6	A	55	0	49	0	0
6	E	55	0	49	0	0
6	I	55	0	49	0	0
7	A	11	0	10	0	0
7	E	11	0	10	0	0
7	I	11	0	10	0	0
All	All	24825	0	24186	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 201 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:VAL:CG1	1:I:121:LYS:H	1.56	1.17
1:E:120:VAL:HG12	1:E:121:LYS:N	1.54	1.17
1:A:120:VAL:HG12	1:A:121:LYS:N	1.54	1.15
1:I:120:VAL:HG12	1:I:121:LYS:N	1.54	1.15
1:A:120:VAL:CG1	1:A:121:LYS:H	1.56	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	19 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	19	59
1	I	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	19	59
2	B	124/145 (86%)	114 (92%)	6 (5%)	4 (3%)	4	24
2	F	124/145 (86%)	113 (91%)	7 (6%)	4 (3%)	4	24
2	J	124/145 (86%)	114 (92%)	6 (5%)	4 (3%)	4	24
3	C	222/224 (99%)	195 (88%)	27 (12%)	0	100	100
3	G	222/224 (99%)	195 (88%)	27 (12%)	0	100	100
3	K	222/224 (99%)	195 (88%)	27 (12%)	0	100	100
4	D	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	31	71
4	H	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	31	71
4	L	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	31	71
All	All	2943/3144 (94%)	2666 (91%)	250 (8%)	27 (1%)	24	59

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	533	ALA
2	B	646	LEU
2	F	533	ALA
2	F	646	LEU
2	J	533	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/420 (94%)	391 (100%)	2 (0%)	90	96
1	E	393/420 (94%)	391 (100%)	2 (0%)	90	96
1	I	393/420 (94%)	391 (100%)	2 (0%)	90	96
2	B	111/125 (89%)	111 (100%)	0	100	100
2	F	111/125 (89%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	111/125 (89%)	111 (100%)	0	100	100
3	C	192/192 (100%)	191 (100%)	1 (0%)	90	96
3	G	192/192 (100%)	191 (100%)	1 (0%)	90	96
3	K	192/192 (100%)	191 (100%)	1 (0%)	90	96
4	D	180/180 (100%)	180 (100%)	0	100	100
4	H	180/180 (100%)	180 (100%)	0	100	100
4	L	180/180 (100%)	180 (100%)	0	100	100
All	All	2628/2751 (96%)	2619 (100%)	9 (0%)	93	98

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	166	ARG
3	K	71	ARG
1	I	127	VAL
3	C	71	ARG
3	G	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	130	GLN
1	E	234	ASN
1	I	234	ASN
1	E	99	ASN
1	I	130	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

105 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	601	1,5	14,14,15	0.68	0	17,19,21	0.50	0
5	NAG	A	602	5,6	14,14,15	0.75	1 (7%)	17,19,21	1.12	1 (5%)
6	BMA	A	603	5,7	11,11,12	1.06	0	15,15,17	1.19	2 (13%)
7	MAN	A	604	6	11,11,12	0.90	0	15,15,17	1.15	2 (13%)
5	NAG	A	605	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	A	606	5	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
5	NAG	A	607	1,5	14,14,15	0.78	0	17,19,21	0.82	1 (5%)
5	NAG	A	608	5,6	14,14,15	0.43	0	17,19,21	2.41	3 (17%)
6	BMA	A	609	5	11,11,12	0.66	0	15,15,17	1.10	1 (6%)
5	NAG	A	610	1,5	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
5	NAG	A	611	5,6	14,14,15	0.68	0	17,19,21	2.24	3 (17%)
6	BMA	A	612	5	11,11,12	0.73	0	15,15,17	0.89	0
5	NAG	A	613	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	4 (23%)
5	NAG	A	614	1,5	14,14,15	0.30	0	17,19,21	0.65	0
5	NAG	A	615	5,6	14,14,15	0.68	1 (7%)	17,19,21	0.73	0
6	BMA	A	616	5	11,11,12	0.92	0	15,15,17	1.30	3 (20%)
5	NAG	A	617	1	14,14,15	0.41	0	17,19,21	0.51	0
5	NAG	A	618	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.65	0
5	NAG	A	619	5	14,14,15	0.30	0	17,19,21	0.95	1 (5%)
5	NAG	A	620	1,5	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
5	NAG	A	621	5	14,14,15	0.22	0	17,19,21	0.54	0
5	NAG	A	622	1,5	14,14,15	0.52	0	17,19,21	0.60	0
5	NAG	A	623	5,6	14,14,15	0.36	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	A	624	5	11,11,12	0.50	0	15,15,17	1.35	1 (6%)
5	NAG	A	625	1,5	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
5	NAG	A	626	5	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
5	NAG	A	627	1	14,14,15	0.30	0	17,19,21	0.52	0
5	NAG	A	628	1,5	14,14,15	0.71	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	A	629	5	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	NAG	A	630	1,5	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
5	NAG	A	631	5	14,14,15	0.74	1 (7%)	17,19,21	0.56	0
5	NAG	A	632	1	14,14,15	0.27	0	17,19,21	1.41	1 (5%)
5	NAG	A	633	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	A	634	5	14,14,15	0.29	0	17,19,21	0.72	0
5	NAG	B	701	2	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
5	NAG	E	601	1,5	14,14,15	0.69	0	17,19,21	0.50	0
5	NAG	E	602	5,6	14,14,15	0.75	1 (7%)	17,19,21	1.12	1 (5%)
6	BMA	E	603	5,7	11,11,12	1.05	0	15,15,17	1.19	2 (13%)
7	MAN	E	604	6	11,11,12	0.91	0	15,15,17	1.15	2 (13%)
5	NAG	E	605	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	E	606	5	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
5	NAG	E	607	1,5	14,14,15	0.79	0	17,19,21	0.82	1 (5%)
5	NAG	E	608	5,6	14,14,15	0.43	0	17,19,21	2.41	2 (11%)
6	BMA	E	609	5	11,11,12	0.66	0	15,15,17	1.11	1 (6%)
5	NAG	E	610	1,5	14,14,15	0.62	0	17,19,21	1.06	1 (5%)
5	NAG	E	611	5,6	14,14,15	0.68	0	17,19,21	2.25	3 (17%)
6	BMA	E	612	5	11,11,12	0.73	0	15,15,17	0.89	0
5	NAG	E	613	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	4 (23%)
5	NAG	E	614	1,5	14,14,15	0.31	0	17,19,21	0.65	0
5	NAG	E	615	5,6	14,14,15	0.68	1 (7%)	17,19,21	0.73	0
6	BMA	E	616	5	11,11,12	0.92	0	15,15,17	1.30	3 (20%)
5	NAG	E	617	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	E	618	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.64	0
5	NAG	E	619	5	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
5	NAG	E	620	1,5	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
5	NAG	E	621	5	14,14,15	0.23	0	17,19,21	0.54	0
5	NAG	E	622	1,5	14,14,15	0.53	0	17,19,21	0.60	0
5	NAG	E	623	5,6	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
6	BMA	E	624	5	11,11,12	0.49	0	15,15,17	1.35	1 (6%)
5	NAG	E	625	1,5	14,14,15	0.28	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	626	5	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
5	NAG	E	627	1	14,14,15	0.30	0	17,19,21	0.52	0
5	NAG	E	628	1,5	14,14,15	0.71	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	E	629	5	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
5	NAG	E	630	1,5	14,14,15	0.58	0	17,19,21	1.18	1 (5%)
5	NAG	E	631	5	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
5	NAG	E	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
5	NAG	E	633	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	E	634	5	14,14,15	0.29	0	17,19,21	0.73	0
5	NAG	F	701	2	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
5	NAG	I	601	1,5	14,14,15	0.68	0	17,19,21	0.50	0
5	NAG	I	602	5,6	14,14,15	0.76	1 (7%)	17,19,21	1.12	1 (5%)
6	BMA	I	603	5,7	11,11,12	1.07	0	15,15,17	1.19	2 (13%)
7	MAN	I	604	6	11,11,12	0.89	0	15,15,17	1.15	2 (13%)
5	NAG	I	605	1,5	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	I	606	5	14,14,15	0.45	0	17,19,21	0.83	1 (5%)
5	NAG	I	607	1,5	14,14,15	0.78	0	17,19,21	0.82	1 (5%)
5	NAG	I	608	5,6	14,14,15	0.43	0	17,19,21	2.41	3 (17%)
6	BMA	I	609	5	11,11,12	0.66	0	15,15,17	1.10	1 (6%)
5	NAG	I	610	1,5	14,14,15	0.63	0	17,19,21	1.05	1 (5%)
5	NAG	I	611	5,6	14,14,15	0.67	0	17,19,21	2.25	3 (17%)
6	BMA	I	612	5	11,11,12	0.73	0	15,15,17	0.89	0
5	NAG	I	613	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	4 (23%)
5	NAG	I	614	1,5	14,14,15	0.30	0	17,19,21	0.65	0
5	NAG	I	615	5,6	14,14,15	0.67	1 (7%)	17,19,21	0.73	0
6	BMA	I	616	5	11,11,12	0.91	0	15,15,17	1.30	3 (20%)
5	NAG	I	617	1	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	I	618	1,5	14,14,15	0.61	1 (7%)	17,19,21	0.64	0
5	NAG	I	619	5	14,14,15	0.31	0	17,19,21	0.96	1 (5%)
5	NAG	I	620	1,5	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
5	NAG	I	621	5	14,14,15	0.22	0	17,19,21	0.54	0
5	NAG	I	622	1,5	14,14,15	0.52	0	17,19,21	0.60	0
5	NAG	I	623	5,6	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
6	BMA	I	624	5	11,11,12	0.50	0	15,15,17	1.35	1 (6%)
5	NAG	I	625	1,5	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
5	NAG	I	626	5	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
5	NAG	I	627	1	14,14,15	0.30	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	I	628	1,5	14,14,15	0.70	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	I	629	5	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
5	NAG	I	630	1,5	14,14,15	0.58	0	17,19,21	1.19	1 (5%)
5	NAG	I	631	5	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
5	NAG	I	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
5	NAG	I	633	1,5	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	I	634	5	14,14,15	0.29	0	17,19,21	0.72	0
5	NAG	J	701	2	14,14,15	0.25	0	17,19,21	0.68	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	602	5,6	-	2/6/23/26	0/1/1/1
6	BMA	A	603	5,7	-	2/2/19/22	0/1/1/1
7	MAN	A	604	6	-	0/2/19/22	0/1/1/1
5	NAG	A	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	606	5	-	2/6/23/26	0/1/1/1
5	NAG	A	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	608	5,6	-	5/6/23/26	0/1/1/1
6	BMA	A	609	5	-	1/2/19/22	0/1/1/1
5	NAG	A	610	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	611	5,6	-	4/6/23/26	0/1/1/1
6	BMA	A	612	5	-	2/2/19/22	0/1/1/1
5	NAG	A	613	1	-	5/6/23/26	0/1/1/1
5	NAG	A	614	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	615	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	616	5	-	1/2/19/22	0/1/1/1
5	NAG	A	617	1	-	1/6/23/26	0/1/1/1
5	NAG	A	618	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	619	5	-	3/6/23/26	0/1/1/1
5	NAG	A	620	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	621	5	-	2/6/23/26	0/1/1/1
5	NAG	A	622	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	623	5,6	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	A	624	5	-	2/2/19/22	0/1/1/1
5	NAG	A	625	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	626	5	-	1/6/23/26	0/1/1/1
5	NAG	A	627	1	-	2/6/23/26	0/1/1/1
5	NAG	A	628	1,5	-	3/6/23/26	0/1/1/1
5	NAG	A	629	5	-	3/6/23/26	0/1/1/1
5	NAG	A	630	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	631	5	-	0/6/23/26	0/1/1/1
5	NAG	A	632	1	-	0/6/23/26	0/1/1/1
5	NAG	A	633	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	634	5	-	0/6/23/26	0/1/1/1
5	NAG	B	701	2	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	602	5,6	-	2/6/23/26	0/1/1/1
6	BMA	E	603	5,7	-	2/2/19/22	0/1/1/1
7	MAN	E	604	6	-	0/2/19/22	0/1/1/1
5	NAG	E	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	606	5	-	2/6/23/26	0/1/1/1
5	NAG	E	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	608	5,6	-	5/6/23/26	0/1/1/1
6	BMA	E	609	5	-	1/2/19/22	0/1/1/1
5	NAG	E	610	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	611	5,6	-	4/6/23/26	0/1/1/1
6	BMA	E	612	5	-	2/2/19/22	0/1/1/1
5	NAG	E	613	1	-	5/6/23/26	0/1/1/1
5	NAG	E	614	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	615	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	616	5	-	1/2/19/22	0/1/1/1
5	NAG	E	617	1	-	1/6/23/26	0/1/1/1
5	NAG	E	618	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	619	5	-	3/6/23/26	0/1/1/1
5	NAG	E	620	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	621	5	-	2/6/23/26	0/1/1/1
5	NAG	E	622	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	623	5,6	-	3/6/23/26	0/1/1/1
6	BMA	E	624	5	-	2/2/19/22	0/1/1/1
5	NAG	E	625	1,5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	626	5	-	1/6/23/26	0/1/1/1
5	NAG	E	627	1	-	2/6/23/26	0/1/1/1
5	NAG	E	628	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	629	5	-	3/6/23/26	0/1/1/1
5	NAG	E	630	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	631	5	-	0/6/23/26	0/1/1/1
5	NAG	E	632	1	-	0/6/23/26	0/1/1/1
5	NAG	E	633	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	634	5	-	0/6/23/26	0/1/1/1
5	NAG	F	701	2	-	2/6/23/26	0/1/1/1
5	NAG	I	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	602	5,6	-	2/6/23/26	0/1/1/1
6	BMA	I	603	5,7	-	2/2/19/22	0/1/1/1
7	MAN	I	604	6	-	0/2/19/22	0/1/1/1
5	NAG	I	605	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	606	5	-	2/6/23/26	0/1/1/1
5	NAG	I	607	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	608	5,6	-	5/6/23/26	0/1/1/1
6	BMA	I	609	5	-	1/2/19/22	0/1/1/1
5	NAG	I	610	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	611	5,6	-	4/6/23/26	0/1/1/1
6	BMA	I	612	5	-	2/2/19/22	0/1/1/1
5	NAG	I	613	1	-	5/6/23/26	0/1/1/1
5	NAG	I	614	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	615	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	616	5	-	1/2/19/22	0/1/1/1
5	NAG	I	617	1	-	1/6/23/26	0/1/1/1
5	NAG	I	618	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	619	5	-	3/6/23/26	0/1/1/1
5	NAG	I	620	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	621	5	-	2/6/23/26	0/1/1/1
5	NAG	I	622	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	623	5,6	-	3/6/23/26	0/1/1/1
6	BMA	I	624	5	-	2/2/19/22	0/1/1/1
5	NAG	I	625	1,5	-	1/6/23/26	0/1/1/1
5	NAG	I	626	5	-	1/6/23/26	0/1/1/1
5	NAG	I	627	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	628	1,5	-	3/6/23/26	0/1/1/1
5	NAG	I	629	5	-	3/6/23/26	0/1/1/1
5	NAG	I	630	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	631	5	-	0/6/23/26	0/1/1/1
5	NAG	I	632	1	-	0/6/23/26	0/1/1/1
5	NAG	I	633	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	634	5	-	0/6/23/26	0/1/1/1
5	NAG	J	701	2	-	2/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	602	NAG	O5-C1	-2.74	1.39	1.43
5	E	602	NAG	O5-C1	-2.72	1.39	1.43
5	A	602	NAG	O5-C1	-2.72	1.39	1.43
5	E	613	NAG	C1-C2	2.48	1.56	1.52
5	A	613	NAG	C1-C2	2.46	1.56	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	611	NAG	C2-N2-C7	7.87	134.20	122.92
5	I	611	NAG	C2-N2-C7	7.86	134.19	122.92
5	A	611	NAG	C2-N2-C7	7.85	134.17	122.92
5	E	613	NAG	C2-N2-C7	7.76	134.04	122.92
5	I	613	NAG	C2-N2-C7	7.74	134.00	122.92

There are no chirality outliers.

5 of 177 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	633	NAG	C8-C7-N2-C2
5	E	633	NAG	O7-C7-N2-C2
5	A	633	NAG	C8-C7-N2-C2
5	A	633	NAG	O7-C7-N2-C2
5	I	633	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	NAG	1	0
5	E	605	NAG	1	0
5	E	633	NAG	1	0
5	I	605	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.